

Supplementary Material

Unveiling the [3+2] Cycloaddition between Difluoromethyl Diazomethane and 3-Ylideneoxindole from the Perspective of the Molecular Electron Density Theory.

Abel Idrice Adjieufack,^{abc*} Vincent Liégeois,^{a*} Ibrahim Ndassa Mbouombouo,^c Luis Ramon Domingo,^{d*} and Benoît Champagne ^{a*}

^a Laboratory of Theoretical Chemistry (LCT) and Namur Institute of Structured Matter (NISM), University of Namur, Rue de Bruxelles, 61, B-5000 Namur, Belgium.

^b Physical and Theoretical Chemistry Laboratory, Faculty of Science, University of Yaoundé I, P.O. Box 812 Yaoundé, Cameroon.

^c Computational Chemistry Laboratory, High Teacher Training College, University of Yaoundé I, P. O. Box 47 Yaoundé, Cameroon.

^d Department of Organic Chemistry, University of Valencia, Dr. Moliner 50, 46100 Burjassot, Valencia, Spain

Email: adjieufack21@gmail.com
vincent.liegeois@unamur.be
luisrdomingo@gmail.com
benoit.champagne@unamur.be

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Table S1. B3LYP/6-31G(d) electronic chemical potential (μ) chemical hardness (η) electrophilicity (ω) and nucleophilicity (N) in eV, in DCM, for DFDAM **1** and 3YOI **2**.

Species	μ	η	ω	N
3YOI 2	-4.27	3.43	2.66	2.81
DFDAM 1	-4.10	4.74	1.77	2.34
DAM 5	-3.62	4.73	1.39	2.81

Table S2. Electronic energies (a.u) computed at the M06-2X/6-311+G(d,p) level for the reactants, TSs and cycloadducts (CAs) involved in this 32CA reaction for different media (gas, solvent)

	gas phase	DCM
1	-386.5079212	-386.5135304
2	-783.5531049	-783.5623325
TS-on	-1170.052290	-1170.064115
TS-ox	-1170.051802	-1170.064282
TS-mn	-1170.048323	-1170.059459
TS-mx	-1170.047483	-1170.059236
3-trans	-1170.120207	-1170.133888
3-cis	-1170.117768	-1170.131589
4-trans	-1170.116532	-1170.131705
4-cis	-1170.118606	-1170.134277

Table S3. Thermodynamics parameters (H° and G° , in a.u and S° , in cal/mol K) for the reactants, TSs and cycloadducts (CAs) involved in the 32CA reaction computed at 25°C and 1 atm with the M06-2X/6-311+G(d,p) method in DCM.

	H°	S°	G°
1	-386.459867	78.9	-386.497378
2	-783.305342	127.9	-783.366127
TS-on	-1169.752169	160.2	-1169.828291
TS-ox	-1169.752324	157.0	-1169.826929
TS-mn	-1169.747675	156.0	-1169.821813
TS-mx	-1169.747442	156.1	-1169.821626
3-trans	-1169.818200	152.3	-1169.890547
3-cis	-1169.815814	150.8	-1169.887462
4-trans	-1169.816127	151.8	-1169.888230
4-cis	-1169.818870	151.5	-1169.890833

Table S4. GDET values evaluated at M06-2X/6-311+G(d,p) as a function of media (Gas and DCM)

	Gas	DCM
TS-on	0.24	0.30
TS-ox	0.24	0.29
TS-mn	0.22	0.25
TS-mx	0.24	0.20

Table S5. Basin Populations (in e) and IRC coordinates (RX, amu^{1/2} Bohr) along the TS-on reaction pathway

Basins	SSD-I		SSD-II		SSD-III		SSD-IV		SSD-V		SSD-VI		SSD-VII		SSD-VIII	
V(N1)	3.75	3.69	3.67	3.55	3.55	3.53	3.53	3.53	3.51	3.50	3.52	3.61	2.93	2.85	2.83	2.69
V'(N1)	-	-	-	-	-	-	-	-	-	-	-	-	0.69	0.80	-	-
V(N1,N2)	3.82	3.83	3.82	3.52	3.42	3.33	3.27	3.27	3.17	3.11	3.05	2.81	2.81	2.74	2.70	2.55
V(N2,C3)	2.94	3.02	3.03	3.44	2.25	2.11	2.01	2.01	1.93	1.89	1.85	1.73	1.74	1.75	1.76	1.82
V(C3,H4)	2.14	2.19	2.52	2.20	2.17	2.15	2.13	2.13	2.12	2.11	2.11	2.06	2.06	2.07	2.06	2.06
V(N2)	-	-	-	-	1.29	1.54	1.74	1.74	1.91	2.05	2.14	2.55	2.58	2.63	2.64	2.71
V(C3)	0.74	0.34	-	-	-	-	-	-	-	-	-	-	-	-	-	-
V'(C3)	0.30	0.57	0.63	0.87	0.90	0.94	0.97	0.97	-	-	-	-	-	-	-	-
V(C4,C5)	3.33	3.32	3.32	3.23	3.22	3.21	2.97	2.97	2.87	2.79	2.55	2.12	2.09	2.07	2.06	1.92
V(C4)	-	-	-	-	-	-	0.21	0.21	-	-	-	-	-	-	-	-
V(C5)	-	-	-	-	-	-	-	-	-	-	0.19	0.43	0.47	0.48	-	-
V(N1,C5)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.39	1.77
V(C3,C4)	-	-	-	-	-	-	-	-	1.30	1.38	1.45	1.82	1.84	1.85	1.86	1.92
RX	25.02	3.52	3.32	0.64	0.32	0.00	-0.32	-0.32	-0.64	-0.96	-1.28	-3.53	-3.85	-4.17	-4.49	-32.06
E(kcal/mol)	28.14	35.21	35.87	43.20	43.80	43.04	43.76	43.76	42.87	41.34	39.24	20.65	18.42	16.21	14.05	0.00

Table S6. Basin Populations (in e) and IRC coordinates (RX, amu^{1/2} Bohr) along the TS-mn reaction pathway

Basins	SSD-I		SSD-II		SSD-III		SSD-IV		SSD-V		SSD-VI		SSD-VII	
V(N1)	3.70	3.74	3.73	3.58	3.55	3.53	3.52	3.55	3.52	3.59	2.93	2.87	2.82	2.75
V'(N1)	-	-	-	-	-	-	-	-	-	-	0.68	0.82	-	-
V(N1,N2)	3.82	3.79	3.81	3.39	3.30	3.19	3.12	3.03	2.98	2.84	2.79	2.69	2.68	2.57
V(N2,C3)	3.06	3.01	3.04	3.54	2.18	1.97	1.92	1.90	1.88	1.83	1.89	1.87	1.86	1.81
V(C3,H4)	2.15	2.18	2.24	2.18	2.18	2.14	2.12	2.10	2.11	2.09	2.09	2.09	2.07	2.05
V(N2)	-	-	-	-	1.47	1.87	2.02	2.09	2.21	2.42	2.48	2.58	2.60	2.71
V(C3)	0.73	0.39	-	-	-	-	-	-	-	-	-	-	-	-
V'(C3)	0.34	0.59	0.60	0.91	0.94	0.96	0.97	0.99	-	-	-	-	-	-
V(C4,C5)	3.36	3.32	3.32	3.21	3.19	3.17	2.95	2.87	2.57	2.30	2.24	2.15	2.10	1.89
V(C4)	-	-	-	-	-	-	-	-	0.26	0.40	0.43	0.51		
V(C5)	-	-	-	-	-	-	0.23	0.29	-	-	-	-	-	-
V(C3,C5)	-	-	-	-	-	-	-	-	1.39	1.56	1.61	1.70	1.74	1.89
V(N1,C4)	-	-	-	-	-	-	-	-	-	-	-	-	1.41	1.75
RX	30.60	5.47	5.15	0.97	0.64	0.00	-0.32	-0.64	-0.97	-1.93	-2.25	-2.90	-3.22	-21.56
E(kcal/mol)	21.92	27.27	27.71	40.54	41.55	42.48	42.20	41.27	39.74	31.73	28.27	20.94	17.33	0.00

Cartesians coordinates (Gas phase) in Ångström

1 (DFDAM)

C	-0.39309300	-0.55383700	0.76735600
N	-1.40902600	-0.13076000	0.07032500
N	-2.27399800	0.26125300	-0.52874700
C	0.95875100	-0.11005000	0.36270600
F	1.38394500	-0.70852200	-0.79427400
H	-0.58724100	-1.27030800	1.54624800
F	0.98070700	1.22750300	0.09923500
H	1.69259500	-0.33065000	1.13768700

2 (3YOI)

C	-2.00557100	2.81880300	-0.00002000
C	-3.29440700	2.29824900	0.00011400
C	-3.51712000	0.91902700	0.00019500
C	-2.40802100	0.09402900	0.00015100
C	-1.08979400	0.59953100	0.00000200
C	-0.89228000	1.97553800	-0.00008500
C	-0.19988200	-0.56477300	-0.00011100
C	-1.11148300	-1.78444000	-0.00005000
C	1.11850900	-0.79607300	-0.00022400
C	2.18907100	0.22184600	-0.00022900
C	4.52467200	0.51295700	-0.00010900
C	5.76567800	-0.34973700	0.00063200
N	-2.40015100	-1.30254100	0.00021600
O	2.04318900	1.41876100	-0.00021200
O	3.39117200	-0.36936600	-0.00026600
O	-0.78492600	-2.94603800	-0.00020300
C	-3.57701000	-2.13931900	0.00008700
H	-1.85973600	3.89154700	-0.00009500
H	-4.14475200	2.96999200	0.00014500
H	-4.52084200	0.51244300	0.00027400
H	0.11017100	2.37653300	-0.00021000
H	4.46670500	1.15409900	0.88205600
H	4.46732400	1.15347900	-0.88276800
H	5.79213600	-0.98592700	-0.88490300
H	6.65488700	0.28292700	0.00083300
H	5.79138200	-0.98538900	0.88658200
H	-4.18119900	-1.95174300	0.89100800
H	-4.18059100	-1.95242500	-0.89139700
H	-3.24253400	-3.17539200	0.00059500
H	1.43845400	-1.83304000	-0.00030000

5 (DAM)

C	-1.14145100	0.00000000	-0.00011800
N	0.15197100	0.00000000	0.00000000
N	1.29795600	0.00000000	0.00000000

H	-1.65044200	-0.95274500	0.00025100
H	-1.65034300	0.95285800	0.00025100

TS-on

C	3.09510300	2.46512000	-1.16853900
C	4.23284800	1.86630800	-0.63833600
C	4.14009100	0.69750600	0.12010400
C	2.88000600	0.16545400	0.32669500
C	1.71163500	0.76038400	-0.19830700
C	1.82731800	1.91740300	-0.95828700
C	0.59735900	-0.08763100	0.23548900
C	1.19364700	-1.20322900	1.02044600
C	-0.78259700	0.04999600	0.30991900
C	-1.46936900	1.29207200	-0.14063500
N	-0.43479200	-1.64478700	-1.65368700
N	2.55231800	-0.99117500	1.03817300
O	-1.24426000	1.87245600	-1.17342800
O	-2.40331200	1.66941600	0.73356300
O	0.60323300	-2.14885800	1.51799400
C	3.50315700	-1.87998500	1.66308800
H	3.19116500	3.36689000	-1.76054700
H	5.20633500	2.30672800	-0.81721700
H	5.02344600	0.22434800	0.53173900
H	0.95001400	2.37739400	-1.39117700
H	4.19877200	-2.28018700	0.92131500
H	4.06630400	-1.35539600	2.43859500
H	2.94151100	-2.69719700	2.11286600
H	-1.25956300	-0.46193600	1.13991000
C	-1.60828600	-1.27248600	-1.11158100
H	-2.24855500	-0.71038700	-1.78608500
C	-2.27367500	-2.35274800	-0.29373400
H	-1.58431800	-2.83124600	0.40527800
F	-3.28053300	-1.75872400	0.39300600
F	-2.83821100	-3.29860500	-1.08958900
N	0.69491400	-1.58741500	-1.60809200
C	-4.14567100	3.08939200	1.50245400
H	-4.73650300	3.98024800	1.28303500
H	-4.82124300	2.23864700	1.59894600
H	-3.63400200	3.23756800	2.45410400
C	-3.14777100	2.85324900	0.39269800
H	-3.63262000	2.69197700	-0.57234500
H	-2.44718200	3.68321600	0.28218400

TS-ox

C	2.56333300	-2.10001600	2.06606300
C	3.84671500	-1.83603700	1.60119600
C	4.05492700	-0.96973500	0.52612200

C	2.94163800	-0.39290200	-0.05885200
C	1.62856600	-0.65273600	0.39247800
C	1.44564600	-1.50861000	1.47152100
C	0.74032400	0.14305200	-0.46426300
C	1.62120900	0.85928600	-1.43676800
C	-0.62221600	0.14095200	-0.74564900
C	-1.53692600	-0.87969600	-0.16693800
N	-0.26569900	2.28240800	0.72617100
N	2.91564400	0.50082900	-1.12923100
O	-1.54054700	-1.23058100	0.98927700
O	-2.38883900	-1.33811500	-1.08054500
O	1.27869200	1.62870200	-2.31389300
C	4.07878500	1.00381400	-1.82059300
H	2.42437300	-2.77028900	2.90526000
H	4.69959100	-2.30333800	2.07869200
H	5.05291100	-0.75644400	0.16274100
H	0.45271100	-1.70998500	1.84707400
H	4.73325300	1.54112400	-1.12977800
H	4.63642200	0.18457700	-2.28101800
H	3.73008900	1.68525000	-2.59497500
H	-0.88507900	0.48465900	-1.74053000
C	-1.43220700	1.87813300	0.18034600
H	-1.75127900	2.51576400	-0.64138400
C	-2.51334200	1.55717600	1.18200800
H	-2.17839300	0.91041900	1.99268400
F	-3.03988300	2.69396700	1.71008000
F	-3.51325900	0.93973900	0.50159100
N	0.84507500	2.07436100	0.82109500
C	-4.25470800	-2.62959400	-1.78409200
H	-5.02841400	-3.33055000	-1.46649200
H	-4.73760400	-1.74245800	-2.19554900
H	-3.66098700	-3.09999400	-2.56884300
C	-3.38504700	-2.26224100	-0.60441700
H	-3.95039400	-1.77080000	0.19005900
H	-2.87868400	-3.12959200	-0.17689700

TS-mn

C	0.97113600	3.09222400	-1.67537100
C	2.10187800	3.40885100	-0.93247400
C	2.48857900	2.62244400	0.15431300
C	1.70322600	1.52604600	0.46273900
C	0.55148000	1.19152000	-0.27310300
C	0.18856100	1.97818400	-1.35602400
C	0.01189000	-0.05498500	0.33509200
C	0.97490200	-0.39524500	1.45274700
C	-1.30164400	-0.47161200	0.55548300
C	-2.46613100	0.11994700	-0.12292600
N	-0.36571300	-2.20905500	-1.12327700
N	1.91174800	0.60269000	1.49220300

O	-2.45602500	0.62473600	-1.22174000
O	-3.57855200	-0.01798400	0.60909400
O	0.94159000	-1.37858000	2.16493800
C	3.08726600	0.56233200	2.33102900
C	0.78212500	-1.50575500	-1.08759600
N	-1.42607500	-2.25213100	-0.70429800
H	0.69075800	3.71270600	-2.51742000
H	2.69658100	4.27441100	-1.19872100
H	3.37255400	2.86028900	0.73322200
H	-0.68838000	1.73240100	-1.93773100
H	3.98443100	0.44333700	1.71760800
H	3.16647500	1.47758900	2.92100800
H	2.98685400	-0.29225600	2.99781200
H	-1.49856000	-1.02909700	1.46336000
C	1.96892600	-2.28045500	-0.57027400
H	1.76038900	-2.82641600	0.35016500
F	2.42455400	-3.15145200	-1.51041800
F	2.96641100	-1.38787600	-0.34477900
H	0.96694900	-0.92857900	-1.99129000
C	-5.91325700	0.19958100	0.98216200
H	-6.85769400	0.55074100	0.56290800
H	-6.00016100	-0.86790600	1.18856700
H	-5.73519200	0.72231600	1.92278400
C	-4.79021700	0.46332900	0.00549400
H	-4.93771300	-0.05716500	-0.94310100
H	-4.67413400	1.52724300	-0.21089000

TS-mx

C	1.58191800	-1.92364500	2.37275400
C	2.78238000	-2.26865500	1.76514800
C	3.03809900	-1.92020900	0.43790500
C	2.05836500	-1.21894200	-0.24080700
C	0.83714800	-0.85267500	0.35655600
C	0.60022300	-1.21286100	1.67548100
C	0.07163000	-0.10485000	-0.67757800
C	0.94218200	-0.13569200	-1.91524900
C	-1.30030900	-0.01624000	-0.92063900
C	-2.30660000	-0.26378100	0.12149600
N	-0.57127800	2.43250900	-0.51418200
N	2.10927900	-0.77041600	-1.56378200
O	-2.13564400	-0.07321900	1.30586100
O	-3.47335600	-0.66240800	-0.39394800
O	0.68340400	0.33932800	-2.99935200
C	3.21020600	-0.99605600	-2.47185800
C	0.65119300	1.94115000	-0.23523800
N	-1.63047400	2.12918600	-0.81130900
H	1.40068700	-2.20452900	3.40272200
H	3.53223700	-2.81533000	2.32415400
H	3.97090700	-2.18821900	-0.04297000

H	-0.32912700	-0.94415400	2.15741700
H	4.12393400	-0.53816000	-2.08587600
H	3.37618300	-2.06674400	-2.61367900
H	2.94811900	-0.54080600	-3.42553600
H	-1.63161300	-0.03954400	-1.95138100
C	1.04960900	2.04882100	1.21743900
H	0.37329500	1.51068300	1.88447800
F	2.29768000	1.54148600	1.32862100
F	1.10577500	3.34885500	1.61502600
H	1.41507700	2.23744600	-0.95086100
C	-5.76544600	-1.26483100	-0.24545800
H	-6.60982300	-1.41331500	0.42980700
H	-6.03442100	-0.50054500	-0.97562600
H	-5.57508200	-2.19959300	-0.77429000
C	-4.54776400	-0.84194800	0.54369300
H	-4.70655700	0.09860200	1.07523100
H	-4.24982700	-1.59492100	1.27612500

3-trans

C	-3.15765400	0.58983500	1.68327800
C	-3.92372600	-0.34585700	0.99717500
C	-3.33078600	-1.32171700	0.19036000
C	-1.95058400	-1.31241500	0.09309300
C	-1.17016300	-0.36299200	0.75868100
C	-1.76274500	0.58227500	1.57193000
C	0.27382900	-0.62696900	0.43246600
C	0.19103800	-1.87082800	-0.48208100
C	1.13493900	0.47272300	-0.24115900
C	0.43722600	1.81330600	-0.16151300
N	2.14343900	-0.48636300	1.71956500
N	-1.13070100	-2.19184500	-0.62878000
O	0.65554200	2.65655300	0.66553500
O	-0.50838400	1.88765000	-1.09550800
O	1.13745900	-2.42076400	-0.98957900
C	-1.60782000	-3.29509200	-1.43335500
H	-3.64209800	1.32381700	2.31480700
H	-5.00261600	-0.32827200	1.09494000
H	-3.93042600	-2.05857400	-0.32967000
H	-1.15963800	1.30419100	2.11217000
H	-2.15761000	-4.00641400	-0.81320300
H	-2.25770800	-2.93009200	-2.23183600
H	-0.73890200	-3.78700800	-1.86704100
H	1.30252500	0.22619800	-1.28995900
C	2.42423800	0.41454900	0.57742600
H	2.72192900	1.38849500	0.97333100
C	3.58826300	-0.16550600	-0.21024100
H	3.41015900	-1.18717200	-0.55238900
F	3.80452600	0.62611400	-1.29892300
F	4.71263900	-0.13370900	0.53969900

N	1.04594100	-1.02504400	1.65333700
C	-2.71498600	2.51426500	-1.69382000
H	-3.47290200	3.29782600	-1.64097200
H	-2.51554800	2.29323300	-2.74325700
H	-3.10561800	1.61555100	-1.21056400
C	-1.45578400	2.96803000	-0.99126200
H	-1.01459400	3.85645900	-1.44755200
H	-1.63082900	3.17374600	0.06590600

3-cis

C	-2.82267900	1.42840500	1.70967200
C	-3.90567500	0.85408500	1.05458400
C	-3.74382500	-0.24867400	0.21139200
C	-2.46010500	-0.73590100	0.04304800
C	-1.35674100	-0.15074600	0.67249600
C	-1.53203400	0.91987100	1.52765800
C	-0.12753200	-0.91895900	0.27763500
C	-0.70108400	-2.03483900	-0.63029000
C	1.03416700	-0.20666000	-0.46122400
C	1.05094700	1.25872000	-0.08248600
N	1.75102600	-1.62621900	1.33379100
N	-2.05336000	-1.83900300	-0.72013900
O	1.54811200	1.69691900	0.92304700
O	0.37699300	1.98710800	-0.96518800
O	-0.05118900	-2.89011500	-1.17733900
C	-2.93824300	-2.67890400	-1.49667400
H	-2.97978500	2.26759000	2.37552500
H	-4.89917000	1.25803500	1.20829800
H	-4.59251300	-0.70684300	-0.28125100
H	-0.68724400	1.35086500	2.05294900
H	-3.67992900	-3.15015700	-0.84787500
H	-3.44766200	-2.08963400	-2.26243900
H	-2.33088500	-3.44727900	-1.97187900
H	0.92849900	-0.30113800	-1.53978600
C	2.22570700	-1.01152400	0.07118700
H	2.45082200	-1.84121900	-0.60578900
C	3.52457800	-0.26165700	0.31340000
H	3.52662100	0.36140900	1.20439500
F	4.53960400	-1.15581100	0.39830800
F	3.77011300	0.52586000	-0.77445300
N	0.53332800	-1.58652100	1.45074600
C	-0.72757400	3.96564600	-1.67717500
H	-0.89633000	5.02277300	-1.46578900
H	-0.28856300	3.87641300	-2.67156900
H	-1.68967600	3.45109700	-1.67002800
C	0.19026100	3.37696600	-0.63195400
H	1.16874300	3.86046800	-0.61226900
H	-0.23968000	3.43310400	0.37024700

4-trans

C	1.81045400	0.54635200	2.71356400
C	2.26499000	1.75185500	2.19244500
C	1.75200800	2.26865900	0.99810200
C	0.77721400	1.52926600	0.35192400
C	0.31354600	0.31316500	0.86311900
C	0.82140700	-0.18612200	2.04581800
C	-0.71532300	-0.24015600	-0.08687200
C	-0.75940100	0.83164800	-1.19108900
C	-0.38804500	-1.61549700	-0.73798200
C	1.02626000	-2.05581500	-0.42235100
N	-2.27208000	-2.02456100	0.42980400
N	0.12591700	1.81925900	-0.85149300
O	1.33877600	-2.90948400	0.35468000
O	1.87710900	-1.26593600	-1.08338800
O	-1.42943700	0.77891200	-2.19591000
C	0.37790200	2.98623100	-1.66682700
C	-2.07095500	-0.56231800	0.58385400
N	-1.39231500	-2.56563000	-0.22792100
H	2.22313300	0.16944700	3.64067600
H	3.02943100	2.30819500	2.72146000
H	2.10608100	3.21085800	0.59769900
H	0.47662700	-1.13605800	2.44169200
H	0.14379400	3.89609200	-1.11003700
H	1.42415600	3.01020200	-1.98139600
H	-0.26409900	2.92102000	-2.54340900
H	-0.52219000	-1.56477900	-1.82294400
C	-3.28110500	0.17302900	0.02587400
H	-3.47923300	-0.01107700	-1.02923300
F	-4.37181100	-0.16208200	0.75196800
F	-3.07316600	1.50894900	0.20249300
H	-2.04975400	-0.34574900	1.65546900
C	3.97826300	-0.19850000	-1.35824500
H	5.03067400	-0.20089900	-1.06970200
H	3.91442500	-0.30344800	-2.44216400
H	3.54086300	0.75878900	-1.06784700
C	3.25461000	-1.32984600	-0.66573300
H	3.65557500	-2.30957300	-0.93178900
H	3.28211400	-1.22794000	0.42199800

4-cis

C	-0.79322700	0.82222500	-2.90049900
C	-1.42638200	1.95597400	-2.40575000
C	-1.35122700	2.30107600	-1.05255100
C	-0.61316900	1.47413000	-0.22374600
C	0.04161000	0.33742100	-0.71107400
C	-0.05325700	-0.00413000	-2.04612200

C	0.70023600	-0.35501000	0.45555300
C	0.32310900	0.54072500	1.64376200
C	0.25680000	-1.82035900	0.66625200
C	-1.10413500	-2.09106600	0.06009600
N	2.35582400	-1.98582600	-0.11801200
N	-0.42265300	1.58428600	1.15570300
O	-1.34070700	-2.82709500	-0.85094700
O	-1.99752200	-1.29892300	0.66340600
O	0.63530600	0.35176000	2.79358500
C	-0.96151700	2.64028200	1.98258500
C	2.21340300	-0.58482600	0.36159000
N	1.32723100	-2.63430000	0.04616200
H	-0.87632700	0.57165600	-3.95024000
H	-1.99524800	2.58626800	-3.07874900
H	-1.85394500	3.18142600	-0.67072100
H	0.41951700	-0.90517800	-2.42457900
H	-0.58079700	3.61034200	1.65577400
H	-2.05342900	2.64312600	1.93533300
H	-0.64426200	2.45090600	3.00654200
H	0.24241000	-2.05721800	1.73709300
C	2.97316500	0.37135900	-0.53151900
H	2.72539100	0.28884400	-1.59051800
F	2.69985400	1.64226600	-0.12226600
F	4.30249500	0.17319000	-0.38163300
H	2.66519200	-0.54242100	1.36102200
C	-4.03810400	-0.09389900	0.73723500
H	-5.02417400	0.03175100	0.28710900
H	-4.16460000	-0.33795500	1.79287500
H	-3.49638700	0.85048400	0.65442700
C	-3.28146600	-1.18813000	0.02075300
H	-3.78752100	-2.15355200	0.07697600
H	-3.11140800	-0.94727200	-1.03194800